

# Metal Hydrides – Science Needs

- **TRADITIONAL METALLIC HYDRIDES: 1.5 to 2 wt.% H. Well studied.**
- **COMPLEX HYDRIDES: 10 to 18 wt.% H with light elements (B, Al).  
Basic science knowledge minuscule.**
- **NEEDED:**
  - ◆ Synthesis of new materials with 10+ wt.% H total
  - ◆ Characterization of crystalline, nanocrystalline and amorphous structures
  - ◆ Methods of self-assembly of  $[\text{MH}_4]^{1-}$  and  $[\text{MH}_6]^{3-}$  complexes (REVERSIBILITY)
  - ◆ Chemical bonding – electronic structure determinations
  - ◆ Structure – property relationships
  - ◆ Hydrogen transport, phase transformations, paths and mechanisms
  - ◆ Detailed theoretical models
  - ◆ Close collaboration between experimental and computational scientists

- **70's and 80's: productive research program:**
  - ◆ Hydrogen storage, embrittlement and diffusion
  - ◆ Electronic structure
  - ◆ Optical characterization, electrotransport
  - ◆ Phase transformations, theory
- **90's to present: internally funded research**
  - ◆ Mechanochemistry of  $\text{LiAlH}_4$ ,  $\text{LiMg}(\text{AlH}_4)_3$ , and others
  - ◆ 7+ wt.% H (~5 wt.% at room temperature and below; ~2.5 wt.% below 150°C)
  - ◆ Solvent-free preparation:  $\text{AlH}_3$  - 10 wt.%  $\text{H}_2$ ;  $\text{LiMg}(\text{AlH}_4)_3$  - 9.7 wt.%  $\text{H}_2$
  - ◆ Preliminary mechanism of the dehydrogenation of Ti-activated  $\text{LiAlH}_4$ .
  - ◆ *In situ* high resolution solid state NMR of nanocrystalline/amorphous hydrides

# Virtual Center for Metal Hydrides

## 1 – Needs

- **Required to coordinate systematic and broad effort to resolve basic science issues**
- **Need to build on strong existing research efforts**
- **Need ability to quickly involve groups with specialized expertise and tools**
- **Need to focus on hydrogen-rich metal hydrides**
- **Need to involve a strong theory/computational component**
- **Need to have a clear path to relevancy**
- **Need well developed mechanisms for technology transfer**

# Virtual Center for Metal Hydrides

## 2 – Case for Ames



- **Materials Preparation Center – DOE user facility**
  - ◆ **State-of-the-art materials preparation, processing and characterization**
- **Strong DOE Research Programs with traditions in metal hydride research**
  - ◆ **Metal and Ceramic Sciences**
  - ◆ **Condensed Matter Physics**
  - ◆ **Materials Chemistry**
  - ◆ **Chemical and Biological Sciences**
- **Located on campus of Tier 1 Research University (Iowa State)**
  - ◆ **Involvement of good undergraduate and graduate students**
  - ◆ **Easy access to experts in engineering, chemistry and other departments**

- **In charge of Beamline at the Advanced Photon Source for structure/property characterization**
- **In charge of Neutron Scattering Spectrometer Facility at the High Flux Isotope Reactor**
- **Ames Laboratory has sister research centers at Iowa State University for tech transfer and industrial outreach**
  - ◆ **Center for Sustainable Environmental Technologies**
  - ◆ **Center for Nondestructive Evaluation**
  - ◆ **Center for Catalysis**
  - ◆ **Center for Physical and Computational Mathematics**
  - ◆ **Center for Advanced Technologies Development**
- **Iowa Energy Center – funded by the State of Iowa**
  - ◆ **Strong interest in renewable energy and hydrogen as a fuel**
  - ◆ **Located in Ames and operated by Iowa State University**